

Glycine, N-benzoyl-, trimethylsilyl ester

Other names:

Hippuric acid, trimethylsilyl ester
Hippuric acid, mono-TMS
Hippuric acid, TMS, #2
Hippuric acid, tms derivative

Inchi:

InChI=1S/C12H17NO3Si/c1-17(2,3)16-11(14)9-13-12(15)10-7-5-4-6-8-10/h4-8H,9H2,1-3

InchiKey:

BKKRGGGOJGSDXNW-UHFFFAOYSA-N

Formula:

C12H17NO3Si

SMILES:

C[Si](C)(C)OC(=O)CNC(=O)c1ccccc1

Mol. weight [g/mol]:

251.35

CAS:

2078-24-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.40		Crippen Method
logp	1.794		Crippen Method
rinpol	1804.00		NIST Webbook
rinpol	1835.00		NIST Webbook
rinpol	1802.00		NIST Webbook
rinpol	1853.00		NIST Webbook
rinpol	1846.00		NIST Webbook
rinpol	1806.00		NIST Webbook
rinpol	1796.00		NIST Webbook
rinpol	1851.00		NIST Webbook
rinpol	1863.10		NIST Webbook
rinpol	1860.50		NIST Webbook
rinpol	1805.00		NIST Webbook
rinpol	1796.00		NIST Webbook
rinpol	1822.00		NIST Webbook
rinpol	1844.00		NIST Webbook
rinpol	1863.10		NIST Webbook
rinpol	1822.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2078242&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/56-558-1/Glycine-N-benzoyl-trimethylsilyl-ester.pdf>

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